Modeling and Measurements for Light Scattering from Smooth Surfaces

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Introduction
Motivation
Instrumentation
Light scattering theory
Examples
Differentiating roughness from other types of defects
Measuring the roughness of two interfaces
☐ Sizing particulate contaminants
□ Paints
Summary



Main Focus of Program

Industry Needs:

- ➤ Optical Scattering for Wafer Surface Inspection
- Extracting as much information from light scatter as possible: Size, shape, composition, location, etc.

Program Strategy:

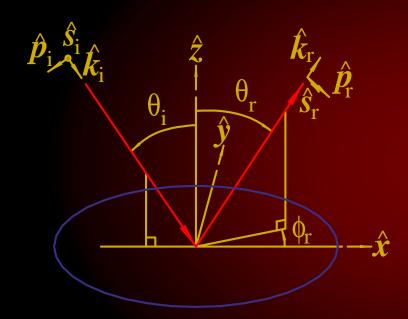
- ➤ To develop a more complete understanding of the physics of light scattering from features on surfaces, and
- ➤ To transfer that understanding to the development of new methodologies that improve defect sensitivity and classification.

Spin-off:

➤ Many of the theoretical models and experimental methods work surprisingly well for some highly scattering media.

Bidirectional Reflectance Distribution Function (BRDF)

$$f_r(\theta_i, \phi_i; \theta_r, \phi_r) = \frac{1}{P_i \cos \theta_r} \frac{\partial P_r}{\partial \Omega}$$



White diffuse materials: $f_r \sim (1/\pi) \text{ sr}^{-1} = 0.32 \text{ sr}^{-1}$

Smooth surfaces: $10^{-9} \text{ sr}^{-1} < f_r < 10^{-3} \text{ sr}^{-1}$ (at large angles)

Polarimetric properties of the scattered light



Goniometric Optical Scatter Instrument

- Dynamic range: 16 decades (in sr⁻¹)
- Wavelengths: 325, 442, 532, and 633 nm
- Full polarimetric capabilities
- Rayleigh-scatter-limited instrument signature
- Nearly any incident/scattering directions
- Housed in Class 10 clean facility
- Well-characterized measurement tool

Workhorse instrument for:

Research

Calibrations

Models

Roughness

Small scale: First-order vector perturbation theory

Large scale: Specular point (facet) theory

Subsurface Features

Rayleigh subsurface defect model

Subsurface specular point (flake) model

Particulate Contaminants

Rayleigh double-interaction model

Mie double interaction model

Discrete dipole approximation

Finite-element time-domain calculation

All of these models have been or can be extended to multiple interfaces (dielectric coatings).

First-Order Vector Perturbation Theory

(assumes small amplitude roughness and small slopes)

Match boundary conditions at interface:

$$\hat{\mathbf{n}}(\mathbf{x}) \times \Delta \mathbf{E}[z(\mathbf{x})] = 0$$
$$\hat{\mathbf{n}}(\mathbf{x}) \times \Delta \mathbf{H}[z(\mathbf{x})] = 0$$

Air (index 1)

Substrate (index n_s+ik_s)

BRDF

Power spectral density (PSD) of surface height function

$$f_r(\theta_i, \theta_r, \phi_r) = (16\pi^2/\lambda^4)\cos\theta_i\cos\theta_r \left[Q(\theta_i, \theta_r, \phi_r)\right] \left|Z(\mathbf{q})\right|^2$$

Polarization factors (which look like Fresnel coefficients)

Spatial wavevector **q** related to scattering angles by Bragg relationship:

$$q_x = k(\sin \theta_r \cos \phi_r - \sin \theta_i)$$
$$q_y = k \sin \theta_r \sin \phi_r$$

Specular Point (Facet) Theory

(assumes surface scattering results from specular reflection from aligned facets)

Fresnel reflection

Air (index 1)

Substrate (index n_s+ik_s)

BRDF

Surface slope distribution function

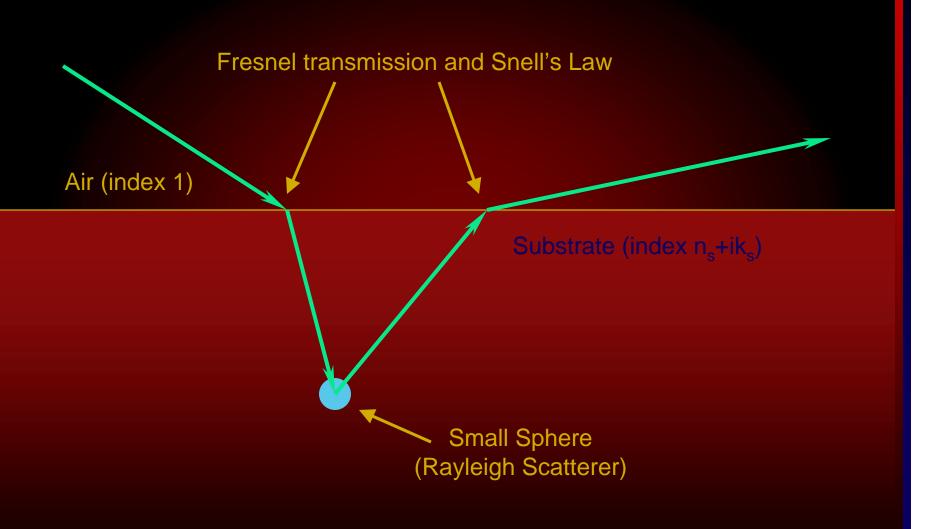
$$f_r(\theta_i, \theta_r, \phi_r) = (1 + s^2)^2 / (4\cos\theta_i \cos\theta_r) R(\theta_i, \theta_r, \phi_r) p(s)$$

Polarization factors

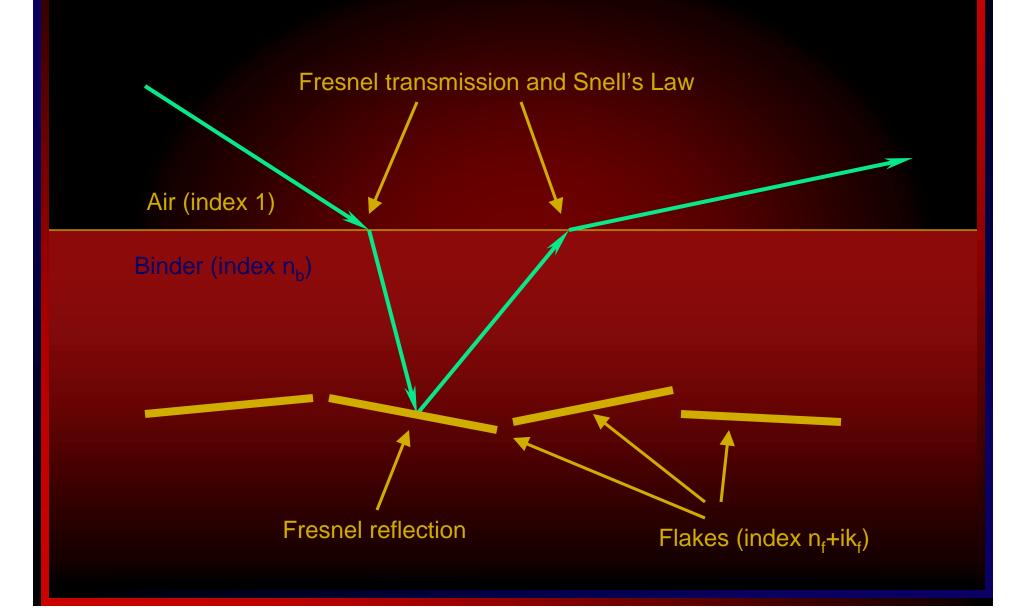
Slope *s* related to scattering angles by:

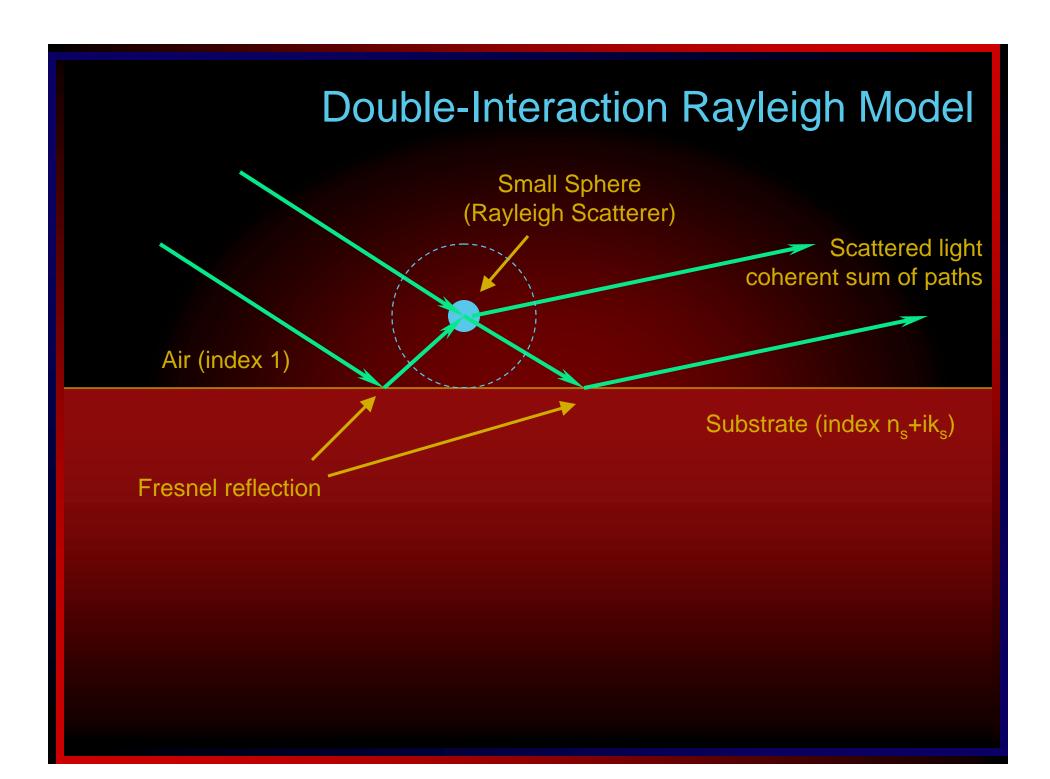
$$s = \frac{\sqrt{\sin^2 \theta_i - 2\sin \theta_i \sin \theta_r \cos \phi_r + \sin^2 \theta_r}}{\cos \theta_i + \cos \theta_r}$$

Subsurface Rayleigh Model

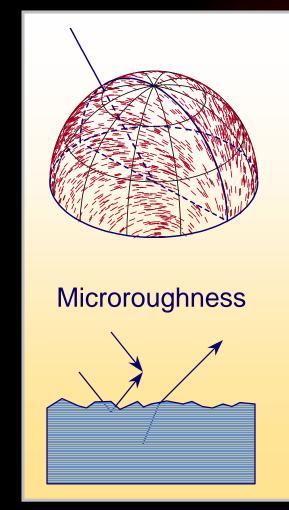


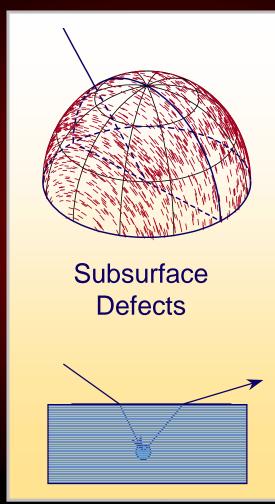
Subsurface Specular Point (Flake) Model

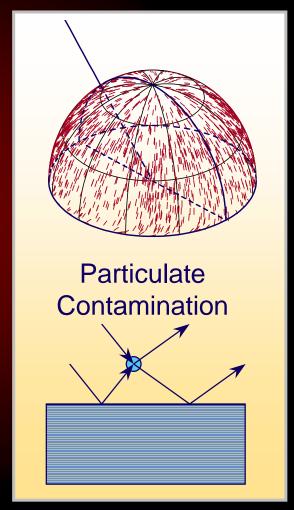




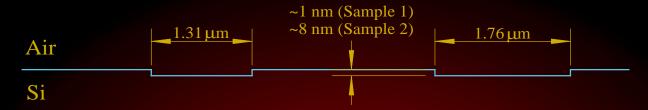
Polarization of light scattered by silicon in the Rayleigh limit for *p*-polarized incident light

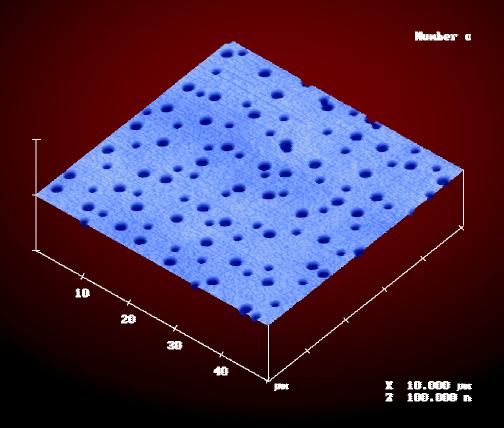






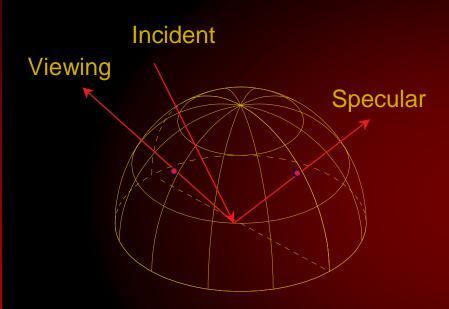
Silicon Microroughness Sample



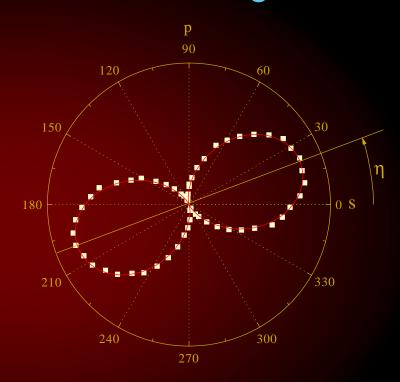


Collaboration with VLSI Standards, Inc.

Polarization of light scattered from photolithographically-produced microrough silicon



$$\theta_i = \theta_r = 45^{\circ}$$
 $\phi_r = 90^{\circ}$
 45° -polarized incident



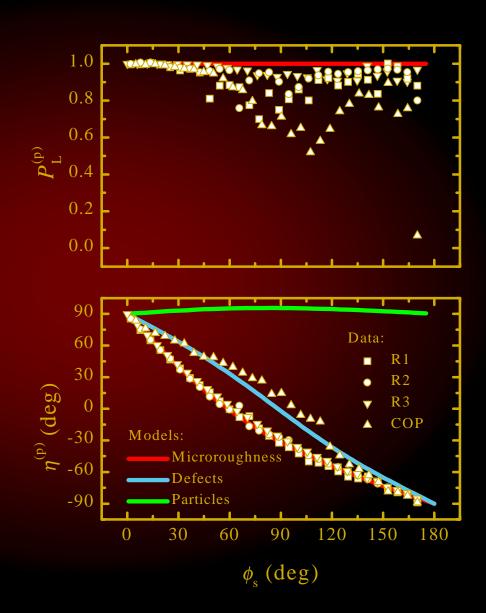
 η = angle from s-polarized $P_{\rm L}$ = degree of linear polarization $P_{\rm C}$ = degree of circular polarization P = degree of polarization

Scattering Ellipsometry of Silicon Wafers

Surface microroughness can be distinguished from subsurface defects and particulate contaminants.

Since the light from roughnesss is polarized in a well-defined direction, one can make a device which is "blind" to microroughness.

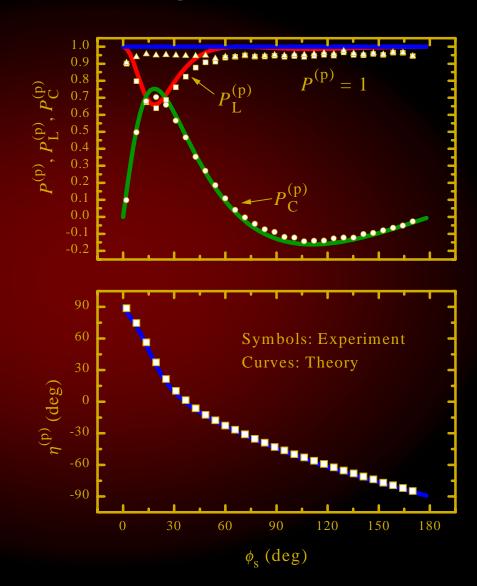
p-polarized incident light $\theta_i = \theta_s = 45^\circ$



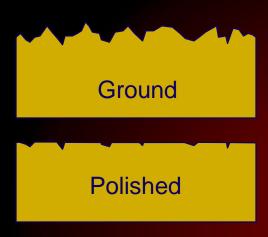
Scattering Ellipsometry of Rough Titanium Nitride

Metallic sample gives rise to elliptical polarization.

p-polarized incident light $\theta_{\rm i}=\theta_{\rm s}=60^{\circ}$ $\lambda=532$ nm

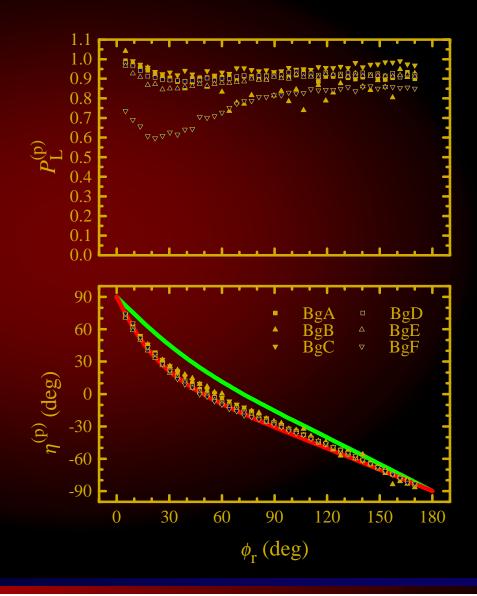


Scattering Ellipsometry of Ground and Polished UG1 Black Glass



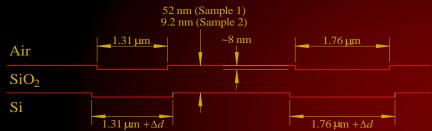
Can we separate roughness from subsurface damage?

p-polarized incident light $\theta_i = \theta_s = 45^\circ$. $\lambda = 532 \text{ nm}$



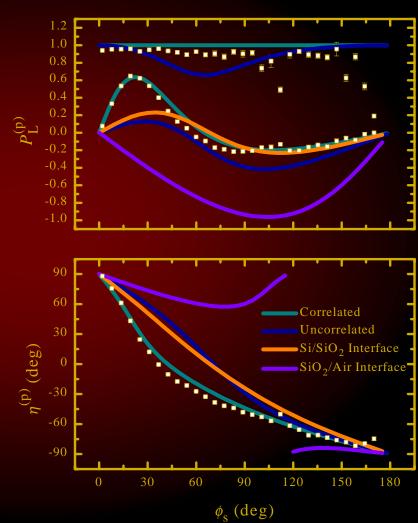
52 nm SiO₂ layer grown on microrough silicon

Sample developed to test roughness scattering from a dielectric film:



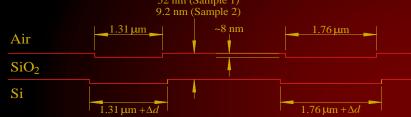
Polarization indicates scattering from correlated roughness but agreement is far from good.

p-polarized incident light $\theta_i = \theta_s = 60^\circ$. $\lambda = 532 \text{ nm}$

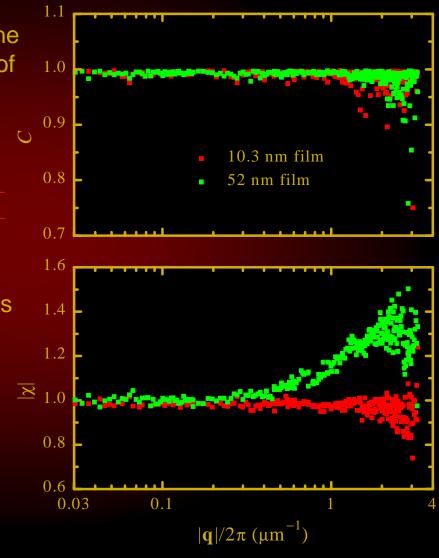


Angle-resolved scattering ellipsometry extends optical measurements of roughness to two interfaces

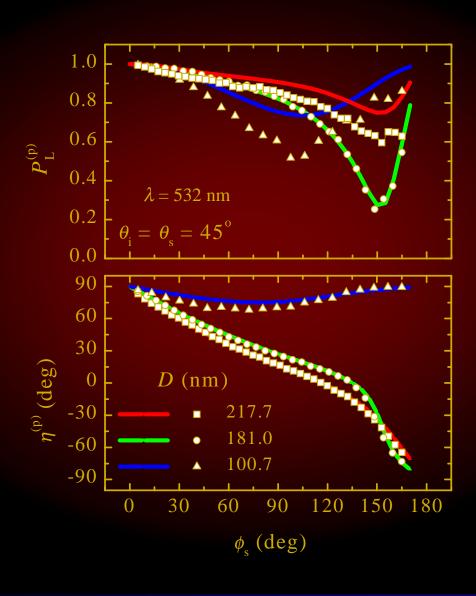
The amplitude of the roughness of the buried interface is smaller than that of the top interface, yet they are correlated with each other.



- Improvements in the inspection of materials with dielectric films requires an understanding of the noise sources, such as roughness.
- Buried interface roughness sheds light on growth mechanism and affects dielectric breakdown and carrier transport properties.



Polystyrene Latex Spheres on Silicon



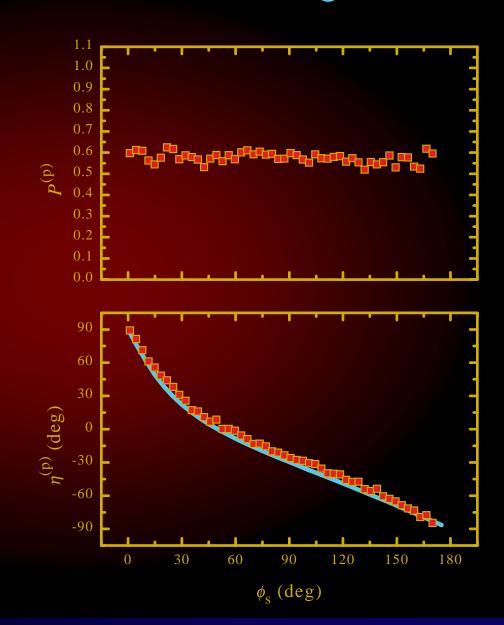
Flat Camouflage Paint

High degree of depolarization, BUT

That part which is polarized follows facet scattering model.

Scattered light is sum of diffuse multiply scattered light plus front surface (facet) scattering.

p-polarized incident light $\theta_i = \theta_s = 45^\circ$. $\lambda = 633 \text{ nm}$

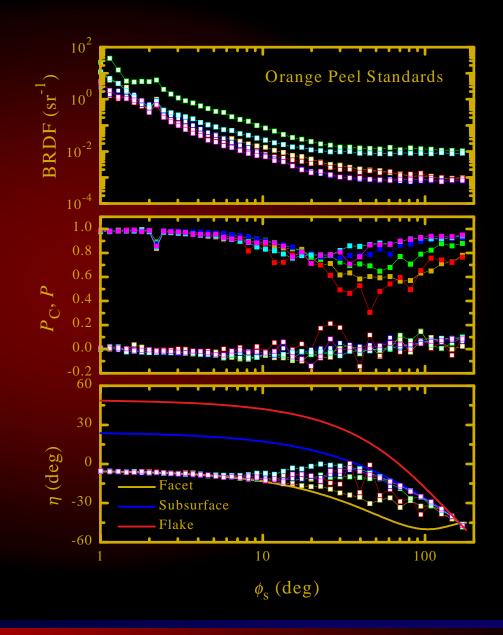


Orange Peel Standards

Black gloss paints with different long-wavelength surface finishes.

Results show capability of differentiating between surface and subsurface scatter.

varying incident light polarization (45° @ ϕ_s = 0° \rightarrow 135° @ ϕ_s = 180°) θ_i = θ_s = 60° λ = 532 nm



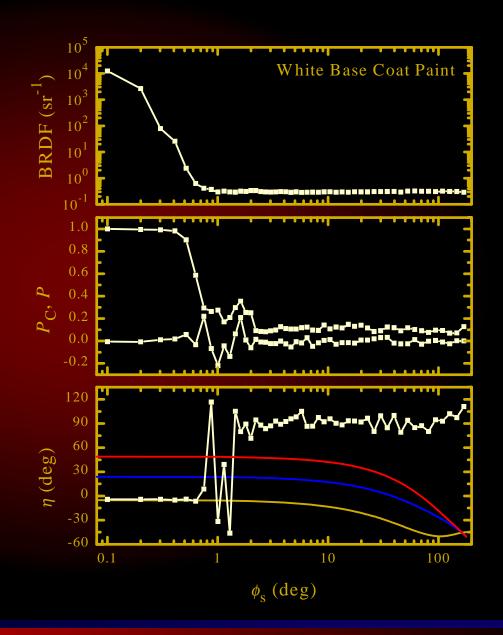
White Base Coat Paint

Glossy white paint.

Results show small angle scatter resulting from front surface reflection and large angle scattering resulting from diffuse multiple scattering.

Diffuse scatter is mostly depolarized with a small p-polarized component resulting from transmission coefficient of light out of binder.

varying incident light polarization (45° @ $\phi_s = 0^\circ \rightarrow 135^\circ$ @ $\phi_s = 180^\circ$) $\theta_i = \theta_s = 60^\circ$ $\lambda = 532 \text{ nm}$



Metallic Paints

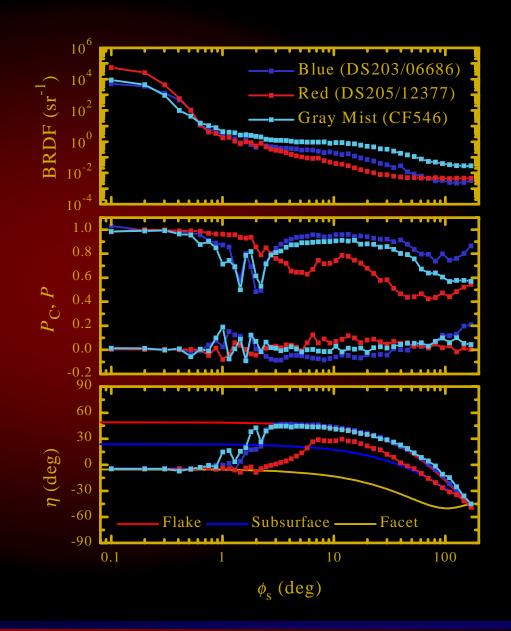
Colored Metallic Paints.

Results of two of the samples show good agreement with metallic flake model.

Metallic flake model requires knowledge of flake material and coatings.

Need characterized samples.

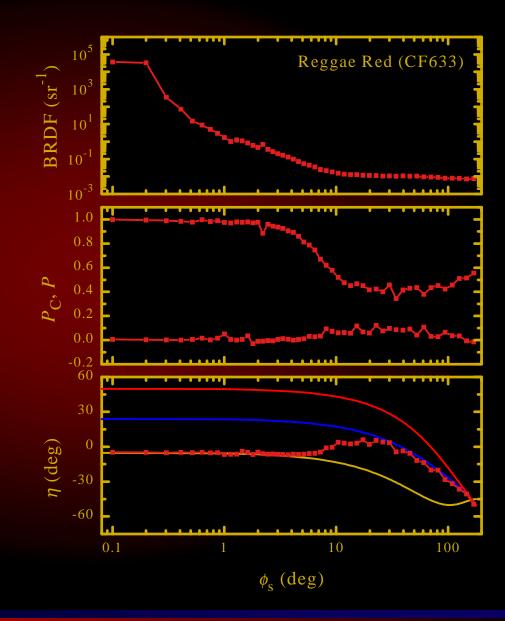
varying incident light polarization (45° @ $\phi_s = 0^\circ \rightarrow 135^\circ$ @ $\phi_s = 180^\circ$) $\theta_i = \theta_s = 60^\circ$ $\lambda = 532 \text{ nm}$



Non-Metallic Red Paint

Results of non-metallic paint shows results similar to orange peel samples.

varying incident light polarization (45° @ $\phi_s = 0^\circ \rightarrow 135^\circ$ @ $\phi_s = 180^\circ$) $\theta_i = \theta_s = 60^\circ$ $\lambda = 532 \text{ nm}$



SCATMECH: Polarized Light Scattering C++ Object Class Library

Originally developed as a tool for organizing and evaluating scattering models and polarimetric quantities.

Contains:

Data types for polarimetric representations

Model-independent base class for all BRDF models

Specific models: Microroughness, Facet, Rayleigh defect, Rayleigh particle, Mie particle, Correlated film microroughness, Lambertian

Applications:

Data-Model comparison

Extracting roughness parameters from data

Polarimetric calculations

Rendering

Available at http://physics.nist.gov/scatmech

Summary

Measurements of the polarization of light scattered by surfaces reveal a large amount of information about sources of scattering. Distinguishing roughness from defects and particulates Extending roughness measurements to multiple interfaces Sizing of particles on surfaces Characterizing scattering sources in paints	
hile this research was focused on issues associated with the emiconductor industry, the applications cross over numerous industry bundaries.	
Inspection of optics, storage media, protective coatings, machined surfaces	
Characterization of polymer films and paint coatings	
Most of the models discussed are available on-line at ☐ http://physics.nist.gov/scatmech.	

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